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Quantum semiconductor devices are playing an increasingly important role in advanced microelectronic applications, including multiple-state logic and memory devices. To model quantum devices, the classical hydrodynamic model for semiconductor devices can be extended to include $O(\hbar^2)$ quantum corrections.

This proposal focused on theoretical and computational investigations of the flow of electrons in semiconductor devices based on the quantum hydrodynamic model. The development of efficient, robuts numerical methods for the QHD model in one and two spatial dimensions wa also emphasized.

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The Quantum Hydrodynamic Model for Semiconductor Devices

Final Report

Carl L. Gardner

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Contents

1 Project Description

1.1 Introduction

Quantum semiconductor devices are playing an increasingly important role in advanced microelectronic applications, including multiple-state logic and memory devices. To model quantum devices, the classical hydrodynamic model for semiconductor devices can be extended to include $O(\hbar^2)$ quantum corrections.

These quantum hydrodynamic (QHD) equations have been remarkably successful in simulating the effects of electron tunneling through potential barriers including single [1, 2] and multiple [3] regions of negative differential resistance in the current-voltage curves of resonant tunneling diodes.

This proposal focused on theoretical and computational investigations of the flow of electrons in semiconductor devices based on the quantum hydrodynamic model. The development of efficient, robust numerical methods for the QHD model in one and two spatial dimensions was also emphasized.

1.2 The QHD model

The QHD model has exactly the same structure [2] as the classical hydrodynamic model (electrogasdynamics):

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_i}(nu_i) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}(mnu_j) + \frac{\partial}{\partial x_i}(u_i mnu_j - P_{ij}) = -n\frac{\partial V}{\partial x_j} - \frac{mnu_j}{\tau_p} \tag{2}$$

$$\frac{\partial W}{\partial t} + \frac{\partial}{\partial x_i}(u_i W - u_j P_{ij} + q_i) = -nu_i\frac{\partial V}{\partial x_i} - \frac{\left(W - \frac{3}{2}nT_0\right)}{\tau_w} \tag{3}$$

$$\nabla\cdot(\epsilon\nabla V) = e^2(N_D - N_A - n) \tag{4}$$

where n is the electron density, $\mathbf{u}$ is the velocity, m is the effective electron mass, P_{ij} is the stress tensor, $V = -e\phi$ is the potential energy, ϕ is the electric potential, $e > 0$ is the electronic charge, W is the energy density, $\mathbf{q}$ is the heat flux, T_0 is the temperature of the semiconductor lattice in energy units (k_B is set equal to 1), ϵ is the dielectric constant, N_D is the density of donors, and N_A is the density of acceptors. Spatial indices i, j equal 1, 2, 3, and repeated indices are summed over. The transport equations (1)–(3) express conservation of electron number, momentum, and energy, respectively, and Eq. (4) is Poisson's equation. The classical collision terms in Eqs. (2) and (3) are modeled by the relaxation time approximation, with momentum and energy relaxation times τ_p and τ_w. The heat flux is specified by Fourier's law $\mathbf{q} = -\kappa \nabla T$, where T is the electron temperature.

Quantum mechanical effects appear in the stress tensor and the energy density. Ref. [2] derives the stress tensor and the energy density for the $O(\hbar^2)$ momentum-shifted thermal equilibrium Wigner distribution function [4]:

$$P_{ij} = -nT\delta_{ij} + \frac{\hbar^2 n}{12m} \frac{\partial^2}{\partial x_i \partial x_j} \log(n) + O(\hbar^4) \tag{5}$$

$$W = \frac{3}{2}nT + \frac{1}{2}mnu^2 - \frac{\hbar^2 n}{24m} \nabla^2 \log(n) + O(\hbar^4). \tag{6}$$

Ancona, Iafrate, and Tiersten [5, 6] derived expression (5) for the stress tensor. In Ref. [1], Grubin and Kreskovsky formulated a one-dimensional version of the QHD equations.

The expansion parameter in the asymptotic series (5) and (6) is actually $\hbar^2/8mTl^2$, where l is a characteristic length scale of the problem [6, 7]. For the resonant tunneling diode in section 1.3 with $T \approx T_0 = 77$ K and $l = 100$ Å, the expansion parameter ≈ 0.23.

There are three major advantages of using the quantum hydrodynamic model over other methods for simulating quantum semiconductor devices. First, the QHD method is much less computationally intensive than the Wigner function [8] or density matrix [9] methods, and includes the same physics if the expansion parameter $\hbar^2/8mTl^2$ is small. Second, the QHD equations are expressed in terms of intuitive classical fluid dynamical quantities (e.g. density, velocity, and temperature). Third, well-understood classical boundary conditions can be imposed in simulating quantum devices.

1.3 Summary of Results

In "The Quantum Hydrodynamic Model for Semiconductor Devices" [2], the full three-dimensional quantum hydrodynamic model is derived for the first time by a moment expansion of the Wigner-Boltzmann equation. The

QHD conservation laws have the same form as the classical hydrodynamic equations, but the energy density and stress tensor have additional quantum terms. These quantum terms allow particles to tunnel through potential barriers and to build up in potential wells.

The 3D QHD transport equations are mathematically classified as having two Schrödinger modes, two hyperbolic modes, and one parabolic mode. The 1D steady-state QHD equations are discretized in conservation form using the second upwind method.

Simulations of a resonant tunneling diode are presented which show charge buildup in the quantum well and negative differential resistance (NDR) in the current-voltage curve. These are the first simulations of the full QHD equations to show NDR in the resonant tunneling diode. The computed current-voltage curve agrees quantitatively with experimental measurements. NDR is interpreted in terms of the time spent by electrons in the quantum well.

The numerical methods and relaxation time models for the QHD model are similar to those for the classical hydrodynamic model. I reported this related work in "Hydrodynamic and Monte Carlo Simulation of an Electron Shock Wave in a One Micrometer $n^+ - n - n^+$ Diode" [10] and in "The ENO Method for the Hydrodynamic Model for Semiconductor Devices" [11], with Joseph Jerome and Chi-Wang Shu. In the first article, hydrodynamic model simulations of a steady-state electron shock wave in a one micrometer Si semiconductor device at 77 K are compared with a Monte Carlo simulation of the Boltzmann equation using the DAMOCLES program. In the second article, the ENO method from computational fluid dynamics is applied to the hydrodynamic model for semiconductor devices. Numerical simulations of a family of steady-state electron shock waves (parametrized by the amount of heat conduction) in a submicron semiconductor device are presented, using the ENO method.

In Ref. [12], the classical (CHD) and quantum hydrodynamic equations are presented in a unified formulation, and results on mathematical classification, upwind discretization, CHD simulations of an electron shock wave, and QHD simulations of NDR in a resonant tunneling diode are summarized.

The phenomenon of resonant tunneling is simulated and analyzed in the QHD model in Ref. [3]. Simulations of a parabolic well resonant tunneling diode at 77 K are presented which show multiple regions of negative differential resistance (NDR) in the current-voltage curve (see Fig. 1). These are

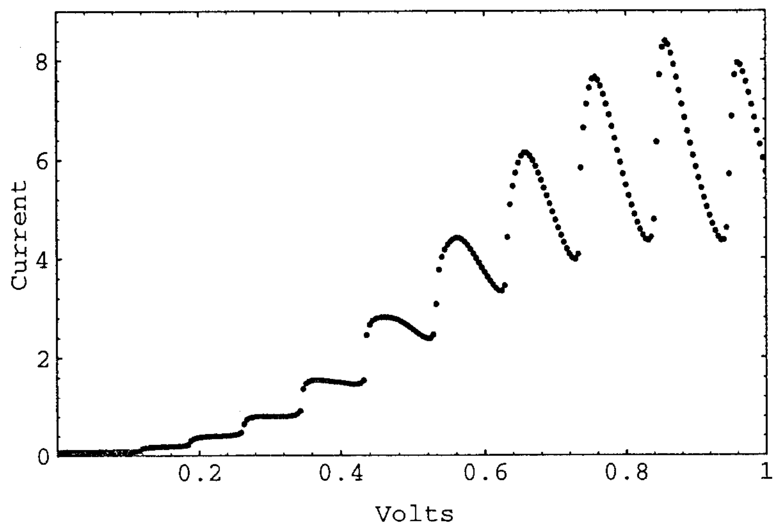

Figure 1: Current density in milliamps/cm^2 vs. voltage for the resonant tunneling diode at 77 K, showing multiple regions of NDR.

the first simulations of the QHD equations to show multiple regions of NDR.

Resonant tunneling (and NDR) depend on the quantum interference of electron wavefunctions and therefore on the phases of the wavefunctions. An analysis of the QHD equations using a moment expansion of the Wigner-Boltzmann equation indicates how phase information is retained in the hydrodynamic equations.

Bistable hysteresis (see Fig. 2) in the current-voltage curve of a resonant tunneling diode is simulated and analyzed in the QHD model in Ref. [13], with Zhangxin Chen, Bernardo Cockburn, and Joseph Jerome. These are the first simulations of the QHD equations to show hysteresis in the current-voltage curve, and confirm that hysteresis is an inherent property of the resonant tunneling diode.

A finite element method for simulation of the time-dependent QHD model is also introduced. The finite element method is based on a Runge-Kutta discontinuous Galerkin (RKDG) method for the QHD conservation laws and a mixed finite element method for Poisson's equation.

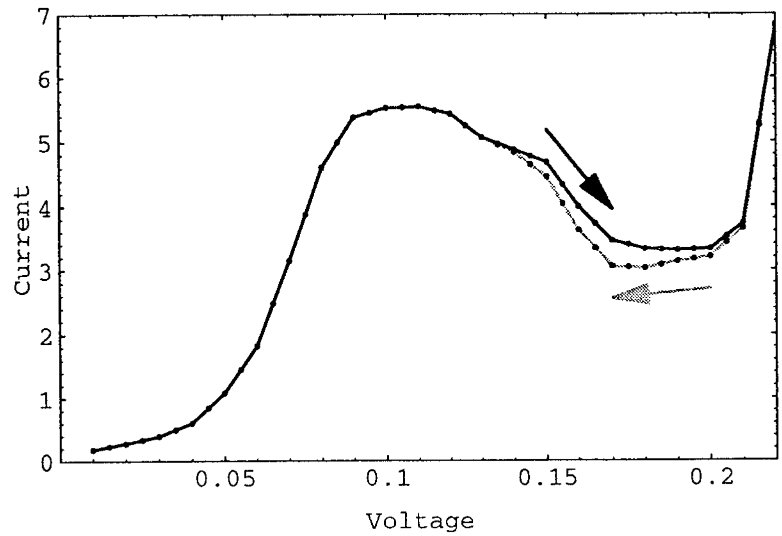

Figure 2: Current density in kiloamps/cm^2 vs. voltage for the resonant tunneling diode at 77 K, showing hysteresis.

1.4 Publications Resulting from this Grant

"Hydrodynamic and Monte Carlo Simulation of an Electron Shock Wave in a One Micron Semiconductor Device," in *Proceedings of the International Workshop on Computational Electronics*, pp. 119–122. Urbana-Champaign: University of Illinois, 1992.

"A New Quantum Hydrodynamic Model for Semiconductor Devices," in *Proceedings of the International Workshop on Computational Electronics*, pp. 313–316. Urbana-Champaign: University of Illinois, 1992.

"Hydrodynamic and Monte Carlo Simulation of an Electron Shock Wave in a One Micrometer $n^+ - n - n^+$ Diode," *IEEE Transactions on Electron Devices* **40** (1993) 455-457.

"The ENO Method for the Hydrodynamic Model for Semiconductor Devices," with J. W. Jerome and C.-W. Shu, in *High Performance Computing, 1993: Grand Challenges in Computer Simulation*, pp. 96–101, San Diego: The Society for Computer Simulation, 1993.

"The Quantum Hydrodynamic Model for Semiconductor Devices," *SIAM Journal on Applied Mathematics* **54** (1994) 409-427.

"The Classical and Quantum Hydrodynamic Models," in *Proceedings of the International Workshop on Computational Electronics*, pp. 25–36. Leeds: University of Leeds, 1993.

"Resonant Tunneling in the Quantum Hydrodynamic Model," accepted for publication in *VLSI Design* (1995).

"Quantum Hydrodynamic Simulation of Hysteresis in the Resonant Tunneling Diode," with Z. Chen, B. Cockburn, and J. W. Jerome, accepted for publication in *Journal of Computational Physics* (1995).

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[13] Z. Chen, B. Cockburn, C. L. Gardner, and J. W. Jerome, "Quantum hydrodynamic simulation of hysteresis in the resonant tunneling diode," *Journal of Computational Physics*, to appear, 1995.